On the Term and Concepts of Numerical Model Validation in Geoscientific Applications

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ABSTRACT

Modelling and numerical simulation of the coupled physical and chemical processes observed in the subsurface are the only options for long-term analyses of complex geological systems. Observations of a certain part of the perceived reality serve as the nucleus of the process of model development. A first step in this process is the establishment of physical models adequately mapping the perceived reality based on decisions to neglect those processes that are not relevant for the considered application. The second step in the definition of process models is the development of a mathematical framework describing the physical model in an approximate manner, and consisting of balance laws and constitutive relations in terms of algebraic, differential or integral equations. Finally, numerical methods and algorithms necessary for a computer-based solution of the process model, and data sets necessary for the numerical simulation constitute the numerical model.

Considering the steps of idealisation and approximation in the course of model development, and the open character of models, Oreskes et al. [3] state that process and numerical models can neither be verified (establishment of the truth of the model), nor validated in general (establishing the legitimacy of a model). Rather the adequacy of models with specific assumptions and parameterisations made during model set-up can be confirmed. If the adequacy of process models with observations can be confirmed using lab as well as field tests and process monitoring, the adequacy of numerical models can be confirmed using numerical benchmarking (e.g., providing analytical solutions) and code comparison for more complex systems [1,2].

Model parameters are intrinsic elements of process and numerical models, in particular constitutive parameters. As they are often not directly measurable, they have to be established by solving inverse problems based on an optimal numerical adaptation of observation results. Within this context, history matching is well-established in geosciences for the parameterisation of complete static site models, whereas stochastic, evolutional or deterministic optimisation approaches are the methods of choice for the parameter identification based on results of lab tests (e.g., uni- or triaxial compression tests).

As modelling cannot provide closed, deterministic predictions, but rather a preview of trends regarding how the studied systems may behave under the defined assumptions and conditions, the solution of inverse problems in geoscientific applications deserves more attention. Within this context, an extensive provision of lab and field test data for an enhanced process understanding combined with a more reliable and documented model calibration are required to improve the adequacy of static and dynamic models. In addition, numerical uncertainty analyses should be an obligatory part of numerical studies for critical real world applications.

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